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Fatty Nitrogen Derived Ether Amines Category High Production Volume (HPV) Chemical Challenge

Assessment of Data Availability and Test Plan

Prepared for:

American Chemistry Council's
Fatty Nitrogen Derivatives Panel
Amines Task Group

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Table of Contents

Introduction 1
Definition of Fatty Nitrogen Derived (FND) Ether Amines Structure-Based Chemical Category 1
Structural Information for the FND Ether Amines Category and Supporting Chemicals 2
Rationale for the FND Ether Amines Structure-Based Chemical Category 3
Available Data to Fulfill HPV Screening Information Data Set (SIDS) Endpoints 5
- Approach to Evaluate the Database for the FND Ether Amines Category 5
- Use of Structure Activity Relationships for the FND Ether Amines Category 6
- Common Features of the Models 6
- Estimation of Physical/Chemical Properties 6
- Estimation of Environmental Fate Properties 6
- Estimation of Environmental Distribution 7
- Estimation of Acute Aquatic Toxicity 7
- Modeling Information Specific to the FND Ether Amine Category 7

Physical/Chemical Properties Data 7
- Summary – Physical/Chemical Properties 9
- Additional Testing – Physical/Chemical Properties 9

Environmental Fate and Ecotoxicity Data 9
- Summary – Environmental Fate and Ecotoxicity 11
- Additional Testing – Environmental Fate and Ecotoxicity 11

Human Health-Related Data 11
- Summary – Human Health-Related Data 14
- Additional Testing – Human Health-Related Studies 14

References 15

List of Tables

Table 1: Structures of FND Ether Amines Category Chemicals 17

Table 2: Physical/Chemical Properties Data for
FND Ether Amines Category Chemicals 21

Table 3: Environmental Fate and Ecotoxicity Data for
FND Ether Amines Category Chemicals 23

Table 4: Human Health-Related Data for FND Ether Amines Category Chemicals 30

Table 5: Proposed Test Plan for American Chemistry Council
FND Ether Amines Category Physical/Chemical Properties.......................................35

Table 6: Proposed Test Plan for American Chemistry Council
FND Ether Amines Category Environmental Fate and Ecotoxicity 37

Table 7: Proposed Test Plan for American Chemistry Council
FND Ether Amines Category Human Health-Related Data...39

Appendices

Appendix A: Robust Summaries for Reliable Studies

Index of Robust Summaries A-1

Physico-chemical Properties Robust Summaries A-34

Environmental Fate Robust Summaries...A-74

Human Health Robust Summaries A-320

Appendix B: Robust Summaries for SAR Model Data

Index of Robust Summaries B-1

Robust Summaries..B-3

Fatty Nitrogen Derived Ether Amines Category
High Production Volume (HPV) Chemicals Challenge
Assessment of Data Availability

Introduction

Surfactants have a long history of use and have been studied extensively for environmental fate and effects, and human health effects. The Fatty Nitrogen Derived (FND) Ether Amines Category chemicals have surfactant properties (e.g. comprised of hydrophobic and hydrophilic ends, form micelles, alter/reduce surface tension, form oil/water emulsions), and are used as additives and in the production of commercial surfactants such as ethoxylated ether amine surfactants. Some typical applications of FND Ether Amines Category chemicals are collectors for flotation process, additives for fuels, lubricants, and petroleum refining, corrosion inhibitors for metalworking fluids, chemical intermediates, textile chemical foaming agents, specialty surfactants, ethoxylates, agricultural chemicals, and cross linking agents for epoxy resins

Definition of Fatty Nitrogen Derived (FND) Ether Amines Structure-Based Chemical Category

The FND Ether Amines Category is comprised of six ether amines with unique Chemical Abstracts Service Registry Numbers (CAS RN; see Text Table A).

The six FND Ether Amines Category chemicals include four long-chain substituted propanamines (CAS RN 68784-38-3, 30113-45-2, 218141-16-3 and 151789-06-9) and two long-chain substituted propanediamines (CAS RN 68479-04-9 and 151789-07-0).

In addition to the FND Ether Amines Category chemicals in the HPV program, two FND ether amines and 22 FND amines are included as supporting chemicals in this data review and Test Plan.

The FND Ether Amines Category chemicals and supporting chemicals are described in the following table. The HPV-sponsored FND Ether Amines chemicals are shaded for ease of identification.

Text Table A: CAS Registry Numbers and Chemical Names

CAS RN	Chemical Name
68784-38-3	1-Propanamine, 3-(C_{8-10}-alkyloxy) derivs.
30113-45-2	1-Propanamine, 3-(isodecyloxy)-
28701-67-9	1-Propanamine, 3-(isodecyloxy)-, acetate
218141-16-3	1-Propanamine, 3-(C_{9-11}-isoalkyloxy)derivs., C_{10} rich
68511-40-0	1-Propanamine, 3-(tridecyloxy)-, branched
151789-06-9	1-Propanamine, 3-(C_{11-14}-isoalkyloxy)derivs., C_{13} rich
68479-04-9	1,3-Propanediamine, N-[3-(tridecyloxy)propyl]-, branched
151789-07-0	1,3-Propanediamine,N-(3-(C11-14-isoalkyloxy)propyl)derivs, C13 rich
124-22-1	Dodecylamine
112-18-5	1-Dodecanamine, N,N-dimethyl
112-75-4	1-Tetradecanamine, N,N-dimethyl

Text Table A: CAS Registry Numbers and Chemical Names

CAS RN	Chemical Name
143-27-1	Hexadecylamine
112-69-6	1-Hexadecanamine, N,N-dimethyl
3151-59-5 + 36505-83-6	Hexadecylamine hydrofluoride (Hetaflur) 9-Octadecen-1-amine hydrofluoride
124-30-1	Octadecylamine
112-90-3	Cis-9-Octadecenylamine
4088-22-6	1-Octadecanamine, N-methyl-N-octadecyl
124-28-7	1-Octadecanamine, N,N-dimethyl
61788-46-3	Amines, coco alkyl
61788-93-0	Amines, coco alkyl dimethyl
61788-62-3	Amines, dicoco alkylmethyl
61791-31-9	Ethanol, 2,2'-iminobis-, N-coco alkyl derivs.
61788-45-2	Amines, hydrogenated tallow alkyl
61788-95-2	Amines, (hydrogenated tallow alkyl)dimethyl
61789-79-5	Amines, bis(hydrogenated tallow alkyl)
61788-63-4	Dihydrogenated tallow methylamine
61790-33-8	Amines, tallow alkyl
61791-55-7	Amines, N-tallow alkyltrimethylenedi-
61791-44-4	Ethanol, 2,2'-iminobis-,N-tallow alkyl derivs.
61788-91-8	Amines, dimethyl soya alkyl

<u>Structural Information for the FND Ether Amines Category and Supporting Chemicals</u>

The following table presents the molecular formula and molecular weight data for the chemicals with defined structures or average molecular weight data for chemicals without defined structures. The structures for these and the remaining chemicals in the FND Ether Amines Category are provided in Table 1.

Text Table B: Molecular Formula and Molecular Weight of FND Ether Amines Category Chemicals Based on Defined or Representative Structures

CAS RN	Name	Molecular Formula	Molecular Weight[a]
68784-38-3	1-Propanamine, 3-(C_{8-10}-alkyloxy) derivs.	$C_{12}H_{27}NO$	201
30113-45-2	1-Propanamine, 3-(isodecyloxy)-	$C_{13}H_{29}NO$	215
28701-67-9	1-Propanamine, 3-(isodecyloxy)-, acetate	$C_{13}H_{29}NO$	215[b]
218141-16-3	1-Propanamine, 3-(C_{9-11}-isoalkyloxy) derivs., C_{10} rich	$C_{13}H_{29}NO$	215
68511-40-0	1-Propanamine, 3-(tridecyloxy)-, branched	$C_{16}H_{35}NO$	257
151789-06-9	1-Propanamine, 3-(C_{11-14}-isoalkyloxy) derivs., C_{13} rich	$C_{16}H_{35}NO$	257
68479-04-9	1,3-Propanediamine, N-[3-(tridecyloxy)propyl]-, branched	$C_{19}H_{42}N_2O$	315
151789-07-0	1,3-Propanediamine,N-(3-(C11-14-isoalkyloxy)propyl)derivs, C13 rich	$C_{19}H_{43}N_2O$	316

Text Table B: Molecular Formula and Molecular Weight of FND Ether Amines Category Chemicals Based on Defined or Representative Structures

CAS RN	Name	Molecular Formula	Molecular Weight[a]
124-22-1	Dodecylamine	$C_{12}H_{27}N$	185
112-18-5	1-Dodecanamine, N,N-dimethyl	$C_{14}H_{31}N$	213
112-75-4	1-Tetradecanamine, N,N-dimethyl	$C_{16}H_{35}N$	241
143-27-1	Hexadecylamine	$C_{16}H_{35}N$	241
112-69-6	1-Hexadecanamine, N,N-dimethyl	$C_{18}H_{39}N$	270
3151-59-5 +36505-83-6	Hexadecylamine hydrofluoride (Hetaflur) 9-Octadecen-1-amine hydrofluoride	$C_{16}H_{35}N.H\text{-}F$ $C_{18}H_{37}N.H\text{-}F$	241[c] 267[c]
124-30-1	Octadecylamine	$C_{18}H_{39}N$	270
112-90-3	Cis-9-Octadecenylamine	$C_{18}H_{37}N$	267
4088-22-6	1-Octadecanamine, N-methyl-N-octadecyl	$C_{37}H_{77}N$	536
124-28-7	1-Octadecanamine, N,N-dimethyl	$C_{20}H_{43}N$	298
61788-46-3	Amines, coco alkyl		200
61788-93-0	Amines, coco alkyl dimethyl		228
61788-62-3	Amines, dicoco alkylmethyl		397
61791-31-9	Ethanol, 2,2'-iminobis-, N-coco alkyl derivs.		302
61788-45-2	Amines, hydrogenated tallow alkyl		263
61788-95-2	Amines, (hydrogenated tallow alkyl)dimethyl		291
61789-79-5	Amines, bis(hydrogenated tallow alkyl)		509
61788-63-4	Dihydrogenated tallow methylamine		523
61790-33-8	Amines, tallow alkyl		262
61791-55-7	Amines, N-tallow alkyltrimethylenedi-		320
61791-44-4	Ethanol, 2,2'-iminobis-,N-tallow alkyl derivs.		364
61788-91-8	Amines, dimethyl soya alkyl		292

Shaded cells indicate HPV-sponsored chemicals.
[a] Average chain length or estimated chain length is used where appropriate; where no formula is provided, the molecular weight is that used by the industry to define the chemical.
[b] Does not include the acetate salt.
[c] Molecular weight of the alkyl chain (excludes the hydrofluoride salt).

Rationale for the FND Ether Amines Structure-Based Chemical Category

The members of the FND Ether Amines Category are large surfactant molecules. As such, they fall into a family of surfactants, all of which have similar physical/chemical properties. The FND surfactants (amines, cationics, amides) employ either defined long-chain alkyl substituents or use natural oils. The following table summarizes the long-chain alkyl substituents found in the FND Ether Amines Category and supporting chemicals:

Text Table C: Chain Length and Degree of Unsaturation for Long-Chain Substituents in the FND Ether Amines Category and Supporting Chemicals

Identifier	Chain Length(s) or Average	Degree of Unsaturation
C8-C10 alkyl	9	None
Isodecyl	10	None
C9-C11 (C10 rich)	10	None

Text Table C: Chain Length and Degree of Unsaturation for Long-Chain Substituents in the FND Ether Amines Category and Supporting Chemicals

Identifier	Chain Length(s) or Average	Degree of Unsaturation
Dodecyl	12	None
Tridecyl	13	None
C11-C14 (C13 rich)	13	None
Tetradecyl	14	None
Hexadecyl	16	None
C14-C18	Not specified	None
C12-C18	Not specified	None
C14-C18 and C16-C18 unsaturated	Not specified	Not specified
C16-C18 and C18-unsaturated	Not specified	Not specified
Octadecyl	18	None
Octadecenyl	18	1
Coco (coconut)	C6: 0-1% C8: 5-9% C10: 5-10% C12: 44-53% C14: 13-19% C16: 8-11% C18: 1-3% C16: 0-1% C18: 5-8% C18: 1-3%	None None None None None None None 1 1 2
Tallow, hydrogenated[1]	C14: 1-6% C16: 23-46% C18: 49-67%	None None None
Tallow	C14: 1-6% C16: 20-37% C18: 14-21% C16: 3-9% C18: 35-46% C18: 4-10% C18: 0-3%	None None None 1 1 2 3
Soya (soy bean)	C16: 7-11% C18: 2-7% C20: 0-2% C18: 20-30% C18: 43-56% C18: 8-14%	None None None 1 2 3

Based on an analysis of data across the FND chemicals, the chain length and degree of unsaturation in the FND surfactants does not appear to have a significant impact on fate and effects. A careful examination of the chemical structures (Table 1) shows the close relationship of all of the HPV and supporting chemicals in the category.

[1] Percentages assume 100% hydrogenation of the unsaturated tallow chains.

The four propanamine derivatives in the Category are similar structurally, with alkyl substituents varying only by approximately 3 carbons, as well as from the perspective of environmental fate and toxicity. The alkyl substituents are C8-C10, C10, a C10 rich mixture of C9-C11, and a C13 rich mixture of C11-C14. The two propanediamine derivatives in the Category are also virtually identical (C13 and C13 rich mixture of C11-C14), have similar environmental fate and toxicity profiles and, except for the addition of the second nitrogen, are essentially the same as the propanamines.

Available Data to Fulfill HPV Screening Information Data Set (SIDS) Endpoints

Approach to Evaluate the Database for the FND Ether Amines Category

The following approach was used to obtain and analyze data relevant to the assessment of the FND Ether Amines Category.

1. The chemical names and CAS RN of six HPV FND Ether Amines Category chemicals supported by the American Chemistry Council Fatty Nitrogen Derivatives Panel, Amines Task Group (Task Group) were provided.
2. The chemicals included in the FND Amines HPV Category with supporting data were included in the FND Ether Amines Category and the Robust Summaries for the FND Amines chemicals were included directly in this submission.
3. As available, published and unpublished reports were obtained from the members of the FND Ether Amines Task Group and reviewed to identify studies that could fulfilled SIDS endpoints.
4. Pertinent databases[2] were searched and all identified relevant reports were obtained to establish the full extent and nature of the published literature for the six FND Ether Amines Category.
5. Each of the reports obtained was reviewed to determine adequacy according to EPA criteria and reliability according to Klimisch *et al.* (1997) and assigned a Klimisch score.
6. Robust summaries were prepared for each report with Klimisch scores of 1 or 2, according to the guidelines proposed by the EPA (U. S. EPA, 1999a) for each study type.
7. Where possible, estimates for physical/chemical properties, environmental fate and ecotoxicity values were developed for the HPV and supporting chemicals by using appropriate Structure Activity Relationships (SAR).
8. Where possible, fugacity modeling was performed to estimate transport and distribution into environmental compartments for the HPV and supporting chemicals.
9. Robust summaries were generated for the SAR data.

[2] Databases include ChemIDplus, HSDB (Hazardous Substances Data Bank), IRIS (Integrated Risk Information System), CCRIS (Chemical Carcinogenesis Research Information System), GENE-TOX, EMIC (Environmental Mutagen Information Center), DART/ETIC (Developmental and Reproductive Toxicology and Environmental Teratology Information Center), MEDLINE, TOXLINE, RTECS (Registry of Toxic Effects of Chemical Substances), TSCATS (Toxic Substances Control Act Test Submissions), and IUCLID, 1996 (International Uniform Chemical Information Database).

Use of Structure Activity Relationships for the FND Ether Amines Category

Approaches recommended in the EPA document on the use of SAR in the HPV Chemicals Challenge Program were employed in the assessment of the FND Ether Amines Category (U. S. EPA, 1999b). Several models were employed to support the review and assessment of the FND Ether Amines Category chemicals. The models included several based on SAR, as well as Mackay-type fugacity-based modeling. The SAR models for physical properties were used to estimate boiling points, melting points, aqueous solubility, octanol-water partition coefficients and vapor pressures. Other SAR models were used to estimate hydroxyl radical mediated atmospheric photo-oxidation and biodegradation potential. SAR models also were used to obtain estimates of acute toxicity to aquatic organisms.

Common Features of the Models

All of the models (except the Mackay-type models) require the input of a molecular structure to perform the calculations. The structure must be entered into the model in the form of a SMILES (Simplified Molecular Input Line Entry System) notation or string. SMILES is a chemical notation system used to represent a molecular structure by a linear string of symbols. The SMILES string allows the program to identify the presence or absence of structural features used by the submodels to determine the specific endpoint. The models contain files of structures and SMILES strings for approximately 100,000 compounds, accessible via CAS RN. SMILES strings cannot be developed for mixtures or chemicals without a single, definable structure.

Estimation of Physical/Chemical Properties

The SAR models for estimating physical properties and abiotic degradation were obtained from Syracuse Research Corporation, 2000 (Estimation Programs Interface for Windows, Version 3.05 or EPIWIN v. 3.05). The models were used to calculate melting point, boiling point, vapor pressure (submodel MPBPVP), octanol-water partition coefficient (K_{ow}) (submodel KOWWIN), and aqueous solubility (submodel WSKOWWIN). The calculation procedures are described in the program guidance and are adapted from standard procedures based on analysis of key structural features (Meylan and Howard, 1999a, b, and c).

Estimation of Environmental Fate Properties

Atmospheric photo-oxidation potential was estimated using the submodel AOPWIN (Meylan and Howard, 2000a). The estimation methods employed by AOPWIN are based on the SAR methods developed by Dr. Roger Atkinson and co-workers (Meylan and Howard, 2000a). The SAR methods rely on structural features of the subject chemical. The model calculates a second-order rate constant with units of cm^3/molecules-sec. Photodegradation based on atmospheric photo-oxidation is in turn based on the rate of reaction (cm^3/molecules-sec) with hydroxyl radicals (HO•), assuming first-order kinetics and an HO• concentration of 1.5 E+6 molecules/cm^3 and 12 hours of daylight. Pseudo first-order half-lives ($t_{1/2}$) were then calculated as follows: $t_{1/2} = 0.693/[(k_{phot} \text{ x HO}\bullet) \text{ x } (12\text{-hr}/24\text{-hr})]$.

The database that supports the modeling of water stability provides only for neutral organic compounds that have structures that can be hydrolyzed. Therefore, no model estimates for hydrolytic stability are available since the FND Ether Amines Category chemicals do not have the necessary characteristics.

Estimation of Environmental Distribution

The Level 3 Mackay-type, fugacity-based models were obtained from the Trent University's Modeling Center. The specific model used was the generic Equilibrium Concentration model (EQC) Level 3, version 1.01. These models are described in Mackay *et al*. (1996a and b). Fugacity-based modeling is based on the "escaping" tendencies of chemicals from one phase to another. For instance, a Henry's Law constant calculated from aqueous solubility and vapor pressure is used to describe the "escape" of a chemical from water to air or vice versa as equilibrium between the phases is attained. The key physical properties required as input parameters into the model are melting point, vapor pressure, K_{ow} and aqueous solubility. The model also requires estimates of first-order half-lives in the air, water, soil and sediment. An additional key input parameter is loading of the chemical into the environment.

Estimation of Acute Aquatic Toxicity

Models developed by the U. S. Environmental Protection Agency (EPA) were employed to make estimates of acute toxicity to aquatic organisms, specifically a commonly tested fish, the fathead minnow (*Pimephales promelas*), a water column dwelling invertebrate (*Daphnia magna*) and a commonly tested green alga, *Selenastrum capricornutum*. The models are incorporated in a modeling package called ECOSAR, version 0.99f (U. S. EPA, 2000). ECOSAR may be obtained from the EPA website for the Office of Pollution Prevention and Toxics, Risk Assessment Division. The models calculate toxicity based on structural features and physical properties, mainly the K_{ow} (Meylan and Howard, 1998).

Modeling Information Specific to the FND Ether Amine Category

When CAS RN were included in the files of structures, the models described above were used for the FND Ether Amines Category chemicals and supporting chemicals. Estimations of physical properties, environmental fate and distribution, and ecotoxicity were not possible for four of the FND Ether Amine Category Chemicals, one of the FND ether amine supporting chemicals and 12 of the FND amine supporting chemicals because they do not have single definable structures and/or were not available in the files of structures of the models. Model predictions were available for two FND Ether Amine Category chemicals, one FND ether amine supporting chemical and 10 FND amine supporting chemicals. The model did not provide estimates of stability in water for this class of chemicals because the model cannot calculate this parameter for chemicals that do not meet the criteria of neutral organic compounds with structures that can be hydrolyzed. Since the FND Ether Amines Category chemicals are considered to be released into wastewater treatment systems consistent with their use patterns, release to soil and air were considered to be minor avenues of entry for FND Ether Amines Category chemicals into the environment. Therefore, for fugacity modeling, all input was assumed to be into surface water using the chemical specific parameters to attain estimates of the chemical distributions between environmental compartments.

Physical/Chemical Properties Data

The available reliable data and SAR estimates for physical/chemical properties of the FND Ether Amines Category chemicals are presented in Table 2. Robust summaries for the reliable studies are provided in Appendix A and Robust Summaries for the SAR data are included in Appendix B. The Test Plan for Physical/Chemical Properties is outlined in Table 5.

Measurement of physical/chemical properties for surfactants is complicated by their behavior in test systems and the environment. For example, measurement of the octanol/water partition coefficient (log K_{ow}) is confounded by the ability of the chemicals to emulsify octanol/water solutions. The resulting values are inaccurate and of limited utility for determining environmental fate and effects. Similarly, measurements such as melting points and boiling points provide minimal information since they do not identify key characteristics of the molecules. The chemicals are non-volatile due to the size of the molecule and hence the determination of a precise value for vapor pressure is difficult and of little practical use.

As described above, where possible, the physical/chemical property estimation program EPIWIN version 3.05 was used to derive estimates. As with actual measurement, prediction of physical/chemical properties for surfactants is complicated. As explained above, the log K_{ow}, a key determinant in the models, is not an appropriate hydrophobicity parameter for reliably predicting environmental behavior of surfactants. The SAR estimates are based on structure and can be made only for substances for which a structure can be defined. Thus, model data were generated for 13 of the 30 HPV and supporting chemicals that have discrete structures.

The available data for physical/chemical properties are summarized below.

Reported melting points for the supporting chemicals ranged from approximately -20°C to 53°C. Model values for the supporting chemicals ranged from approximately 22°C to 93°C; one chemical (CAS RN 4088-22-6) had a predicted melting point much higher than anticipated or believed realistic of 216°C. EPIWIN predicted melting points for the two propanamine derivatives that could be modeled were 51°C and 81°C and predicted that the melting point for the propanediamine derivative was 130°C. Reported boiling points for the supporting chemicals ranged from approximately 200°C to 350°C. Model estimates made for the supporting chemical boiling points ranged from approximately 260°C to 350°C. Again, the boiling point estimate for CAS RN 4088-22-6 was out of range from expected or believed realistic. Decomposition at 348°C was reported for CAS RN 61788-45-2. Boiling point estimates from the model were 278°C and 322°C for the propanamine derivatives and 380°C for the propanediamine derivative.

As expected, based on extensive practical experience with these and similar large organic molecules, the reported and EPIWIN estimated vapor pressures were extremely low across the FND Ether Amines Category HPV and supporting chemicals. The reported and modeled values were all more than two orders of magnitude lower than water. The FND Ether Amines Category chemicals are therefore expected to be essentially nonvolatile, as is generally the case for molecules of this size and complexity.

Predicted or measured log K_{ow} values are of limited practical use for the FND Ether Amines Category chemicals. An inherent property of surfactants is that they accumulate at the interface between hydrophobic and hydrophilic phases rather than equilibrating between the two phases. Therefore, the accurate measurement of the log K_{ow} of any surfactant is notoriously difficult. Even if such measurements were made accurately, the log K_{ow} is not an appropriate value by which to predict the partitioning behavior of the FND Ether Amines Category chemicals in the environment because of the tendency of surfactants to partition at lipid/aqueous interfaces. The EPIWIN estimated values for the octanol/water partition coefficient (log K_{ow}) ranged from approximately 5 to 8 (with a value of 17 for CAS RN 4088-22-6). For supporting chemicals, a range of values from >3.11 to 8.1 was reported for CAS RN 112-90-3, a log Kow of 3.15 was reported for CAS RN 61788-63-4, and a value for CAS RN 61790-33-8 was reported to be 7.5.

Reported water solubility for the supporting chemicals varied from insoluble to slightly soluble. The variable results from these reports indicate the problems with measuring physical properties of surfactant molecules. While poorly soluble, these chemicals may form micelles and suspensions in aqueous systems. Model predictions for water solubility of the HPV chemicals indicate they would be expected to be only slightly soluble.

Summary – Physical/Chemical Properties

Melting points and boiling points are of very limited value in determining the fate and toxicity of surfactant molecules. The available data and model predictions are considered adequate to define the typical ranges for these endpoints. In addition, these types of molecules tend to degrade rather than boil. Consistent with the size and nature of these molecules, measured and modeled vapor pressures are very low, and the FND Ether Amines Category chemicals are considered to be essentially nonvolatile. Measurement and prediction of physical/chemical properties for surfactants are complicated by their behavior in test systems and the environment, and the log K_{ow} is not an appropriate hydrophobicity parameter for reliably predicting environmental behavior. The available values and estimates are considered of very minimal use and additional testing is not warranted. Water solubility estimates varied from slightly soluble to very insoluble. Overall, it is noted that measurement and prediction of physical/chemical properties for surfactants are complicated by their behavior in test systems and the environment, including strong adsorption and absorption properties and surface tension activity. Although predictions vary, the data and knowledge of the chemicals support the conclusion that the FND Ether Amines Category and supporting chemicals behave similarly from the perspective of physical/chemical properties.

Additional Testing – Physical/Chemical Properties

No additional testing (Table 5) is proposed for the Category based on the limited value gained from attempting to refine physical/chemical properties for these types of chemicals and adequate information is available to support the chemical characteristics across the Category.

Environmental Fate and Ecotoxicity Data

The available reliable data and SAR estimates for the environmental fate and effects of the FND Ether Amines Category chemicals are presented in Table 3. Robust summaries for the reliable studies are provided in Appendix A and Robust Summaries for the SAR data are included in Appendix B. The Test Plan for the Environmental Fate and Ecotoxicity Endpoints is summarized in Table 6.

Models for atmospheric photodegradation were used according to EPA guidelines. However, the fugacity models predict virtually no occurrence of the FND Ether Amines Category chemicals in air, which is consistent with the very low vapor pressures. Nonetheless, modeling of the HPV and supporting chemicals indicates that they would be expected to degrade relatively rapidly upon exposure to light ($t_{1/2}$ values ranging from approximately 1.0 to 2.8 hours).

The HYDROWIN model did not provide estimates of stability in water for this class of chemicals because the model cannot calculate this parameter for chemicals that do not meet the criteria of neutral organic compounds with structures that can be hydrolyzed. These types of chemicals generally do not have hydrolysable groups.

An estimation of the transport and distribution of the FND Ether Amines Category chemicals in environmental media (percent in air, water, soil and sediment) following entry into the environment via water is presented in Table 3. Distribution to air and soil were < 1% for all of the chemicals that could be modeled while distribution to the water compartment varied from 5 to 90% with the remainder in the sediment.

For biodegradation, guideline studies and studies similar to guideline studies were available for two of the propanamine derivative chemicals and 16 of the 22 supporting chemicals in this FND Ether Amines Subcategory. The propanamine derivative chemicals, (HPV chemical, CAS RN 30113-45-2 and ether amine supporting chemical, CAS RN 28701-67-9) were inherently degradable in the OECD 301B protocol with 45% and 51% degraded in 28 days, respectively. For the supporting chemicals, in the majority of cases for studies that did not appear to have limited bioavailability due to the poor water solubility and the procedures employed, 28-day degradation rates greater than 50% were attained often reaching "readily" biodegradation criteria (Table 3). Overall, the chemicals in the FND Ether Amines Category have been shown to be either readily biodegradable or to attain degradation close to meeting the "readily biodegradable" criteria. Based on the data for the alkyl diamine, CAS RN 61791-55-7, the propanediamines will also be degradable.

A number of studies evaluating the toxicity of the supporting chemicals to fish were reported. Three assays for the FND amine supporting chemical CAS RN 61788-63-4 indicated substantial differences in the measured toxicity ranging from 23 to > 1000 mg/L. Again, this range shows the complexity of testing these types of chemicals. In the assay that provided no LC_{50} value (i.e. > 1000 mg/L), the test chemical was observed to be insoluble in the test water. It is likely that the range of values represents bioavailability or physical availability (important because many surfactant-like chemicals are known to kill aquatic organisms via a physical rather than chemical mechanism) of the test chemical to the fish. Except where bioavailability questions arose, the reported LC_{50} values ranged from 0.11 to 9.3 mg/L. These findings are consistent with the FND surfactants (cationics, amides, nitriles, ether nitriles) in general and support the conclusion that the FND chemicals are toxic to fish when bioavailable, presumably due to their surfactant properties. The LC_{50} value (0.16 mg/L) for the HPV chemical, CAS RN 68479-04-9, indicates that the FND Ether Amines Category chemicals are also toxic to fish. Acute toxicity to aquatic invertebrates was determined for the HPV chemical, CAS RN 68479-04-9, with a reported LC_{50} of 0.132 mg/L. Similar to the fish testing, a series of studies evaluating toxicity to aquatic invertebrates is available for the supporting chemicals with EC_{50} values ranging between 0.011and 21 mg/L, except where bioavailability questions arose. Acute toxicity to daphnia was confounded by solubility problems and yielded higher than expected EC_{50} values (35.2 and 790 mg/L) for the amine supporting chemical CAS RN 61788-63-4. In addition, a study examining a mixture of the active ingredient (83.5% or 63% of the HPV chemical) with inert materials (e.g. as used in soap) and using two water sources, indicated that river water reduced the toxicity compared to well water (EC_{50} = 60 vs 22 mg/L, respectively) and that the inert ingredients tended to reduce toxicity (EC_{50} = 6.5 mg/L for the 83.5% material vs 22 for the 63% material). Toxicity to aquatic plants for the supporting chemicals indicates that these amine surfactants are highly toxic to algae (E_bC_{50} and E_rC_{50} values ranging from 0.00075 to 0.17 mg/L). The ECOSAR model for cationic surfactants and for some of the aliphatic amines does not predict toxicity to aquatic organisms accurately when the chemicals are poorly soluble or insoluble in water. However, the prediction for acute fish toxicity for one of the chemicals as an aliphatic amine, rather than as cationic surfactant, is similar to the experimental value (0.87 mg/L predicted vs 0.42 mg/L measured for CAS RN 124-22-1). Similar ECOSAR estimates for the HPV chemicals in the Category indicate that these chemicals are expected to be toxic to aquatic organisms similar to the supporting chemicals.

Summary – Environmental Fate and Ecotoxicity

As anticipated in the EPA guidance for HPV chemicals, only model estimates were available for photodegradation and fugacity. The other exclusively modeled value, stability in water, could not be calculated for this category of chemicals although these chemicals do not generally have hydrolysable groups. Atmospheric photodegradation was predicted to be rapid although fugacity models suggested very minimal distribution of these chemicals to the air. Predicted distribution of the chemicals in the environment was to water and sediment compartments based on the assumption that release of the chemicals to the environment is all via water. Extensive biodegradation testing across the Category indicated that the chemicals are biodegradable, often meeting the "readily biodegradable" criteria. No additional biodegradation studies are proposed since there is no pattern or structural properties of the chemicals within the Category to suggest that non-tested chemicals would behave differently. The substantial numbers of studies evaluating the aquatic toxicity of the FND Ether Amine Category chemicals clearly indicate that these surfactants are highly toxic (LC_{50}/EC_{50} values generally < 10 mg/L) to aquatic organisms when bioavailable. Furthermore, this high toxicity is consistent with the large numbers of tests conducted for other FND surfactants (amides, cationics, nitriles, ether nitriles) and for surfactants in general. Therefore, further testing of these chemicals for aquatic toxicity is considered of little or no value in a screening program such as the HPV Chemical Challenge. For the purpose of the program, all of the FND Ether Amine Category chemicals can be considered highly toxic to aquatic species. Overall, the available data support the conclusion that the FND Ether Amines Category chemicals possess similar environmental fate and ecotoxicity across the category.

Additional Testing – Environmental Fate and Ecotoxicity

No additional testing (Table 6) is proposed for the Category. The available model data are adequate for photodegradation, particularly in light of the very limited potential volatility of the FND Ether Amines Category chemicals, as well as for fugacity. These chemicals are not expected to exhibit hydrolysis under normal conditions. Adequate biodegradation data are available to indicate the chemicals in the Category are readily or nearly readily biodegradable. As noted above, additional testing for aquatic toxicity is unwarranted since all of the FND Ether Amine Category chemicals, similar to other surfactants, can be considered highly toxic to aquatic organisms. The available data are considered adequate for the screening purposes of the HPV Chemical Challenge Program.

Human Health-Related Data

The human health effects data for SIDS endpoints of the FND Ether Amines Category chemicals are presented in Table 4. Robust summaries for the reliable studies are provided in Appendix A. The Test Plan for human health related studies is presented in Table 7.

Acute Toxicity: Rat acute oral LD_{50} values for the supporting propanamine derivative, CAS RN 28701-67-9, were approximately 1200 mg/kg (1460 mg/kg for males; 1030 mg/kg/for females) indicating that the chemical possesses slight acute toxicity by the oral route. The oral LD_{50} values for 20 other supporting chemicals ranged from 0.63 to > 15,000 mg/kg. Eight chemicals (14 studies) were evaluated for acute dermal toxicity in the rabbit giving LD_{50} values >1500 mg/kg. One acute inhalation study (CAS RN 61788-46-3) indicated this chemical caused irritation but no lethality at 0.099 mg/L from a one-hour exposure.

Repeat Dose Toxicity: Repeated dose toxicity studies were available for six supporting chemicals. For the mixture of hydrofluoride salts of hexadecylamine and octadecenamine (CAS RN 3151-59-5 + 36505-83-6), a 24-month feeding study in rats and a 2-year gavage study in dogs were available. The NOAEL for both studies was 6.0 mg/kg/day. Non-specific effects on body weight, food consumption, clinical chemistry measurements and organ weights were observed at 30 mg/kg/day in the rat study. Enlarged intestinal lymph nodes with histological evidence of sinusoidal dilation with congestion and fibroplasia were observed at the high dose. Dogs could not tolerate a dose of 30 mg/kg/day and the high dose was reduced to 12 mg/kg/day after five weeks. Effects at the high dose were minimal, primarily related to decreased serum protein throughout the study.

In two chronic two-year dietary studies in rats for CAS RN 124-30-1, the NOAEL was approximately 25 mg/kg/day. In a one-year chronic dietary study in dogs for this chemical, the reported NOAEL was 3.0 mg/kg/day. In this latter study, the occurrence of "foamy" histiocytes in the mesenteric lymph nodes and abnormal appearance of the intestines was recorded.

A 14-day repeated dose skin study in rats with minimal observations was reported with CAS RN 112-90-3. The chemical was irritating at all doses after several days of dosing with the lowest dose of 0.5% showing minimal irritation. No necropsies were performed so this study is considered of supplemental value to establishing the irritant properties of the test chemical.

A series of repeated dose toxicity studies was reported for CAS RN 4088-22-6. In a limited gavage range finding study in rabbits at doses of 100 to 1000 mg/kg/day, the LOAEL was determined to be 100 mg/kg/day based on altered body weights and reduced food consumption. In a 13-week dietary toxicity study in rats at concentrations of 0.15, 0.5, and 1.5% (approximately 130, 375 and 1000 mg/kg/day), the LOAEL was 130 mg/kg/day. This study reported extensive findings of 'foamy macrophages' in the intestinal mucosa and other organs including ovaries. This finding was dose related and occurred at all doses. The lymph nodes in the intestines were enlarged at all doses as well. No NOAEL was, therefore, established. In three studies with repeated dermal exposure of 7 days or 13 weeks duration, no systemic toxicity was observed but skin irritation was prominent at doses of approximately 5 mg/kg/day and above.

For CAS RN 61790-33-8, a 4-week gavage study had a NOAEL of 12.5 mg/kg/day. A number of repeated dose studies have been reported for CAS RN 61791-44-4. The NOAELs for a 90-day dietary study in rats and dogs were approximately 50 mg/kg/day and 13 mg/kg/day, respectively. In the dog study, the higher doses of 40 and 120 mg/kg/day were poorly tolerated with extensive emesis reported. Both of these studies reported the finding of "foamy macrophages" in the intestines of the animals at the higher doses, similar to that reported for the chemicals discussed above. In a second 90-day study with rats, the NOAEL was 12 mg/kg/day based on slightly lower body weights and the presence of "foamy macrophages" at the highest dose of 400 mg/kg/day. In dermal studies of approximately three or four weeks duration and limited numbers of doses, no systemic toxicity was observed but skin irritation was prominent at doses as low as 2 mg/kg/day.

Genetic Toxicity: Bacterial reverse mutation assays for the two supporting propanamine derivatives and for 12 of the other supporting chemicals are available. All were negative for mutagenic responses. In three studies, (CAS RN 112-75-4, 112-69-6 and 124-28-7) only two strains of bacteria were used and the studies do not adequately fulfill the HPV Chemical Challenge Program requirements. However, the results were negative adding support to the large weight of evidence that the FND Ether Amines Category chemicals are unlikely to be mutagenic. In two cases (CAS RN 124-30-1 and 61788-46-3), toxicity was observed for the higher concentrations used in these studies thus limiting the number of concentrations available for evaluation. However, since the criteria for a positive test includes dose response and the concentrations that could be evaluated were as high as could have been tested, these studies are considered adequate. A CHO/HGPRT gene mutation assay, a mouse lymphoma assay, a chromosome aberration assay and an *in vivo* cytogenetics assay were negative for CAS RN 112-90-3. A series of genetic toxicity screening studies with CAS RN 61788-63-4, mouse lymphoma, *in vitro* UDS, and *in vivo* cytogenetics, were all negative. *In vitro* genetic assays for CAS RN 61791-44-4, including a mouse lymphoma study and a UDS assay were negative for mutagenic effects. An *in vitro* chromosomal aberration assay was negative without metabolic activation but was considered positive with metabolic activation. However, *in vivo* mouse micronucleus and cytogenetics studies were negative indicating the finding in the *in vitro* assay was aberrant. An *in vivo* mouse micronucleus assay for supporting chemical, CAS RN 112-18-5 and an *in vivo* rat micronucleus assay for CAS RN 61790-33-8 were negative. Overall these studies are consistent with evidence showing the lack of mutagenicity for the chemicals in the FND Ether Amines Category as well as the other FND Category chemicals (amides, cationics, nitriles).

Reproductive/Developmental Toxicity: Evaluations of potential reproductive effects were available for five supporting chemicals. For the mixture of hydrofluoride salts of hexadecylamine and octadecenamine (CAS RN 3151-59-5 + 36505-83-6), in a Segment I, reproductive screening assay, male body weights were decreased at the highest dose (30 mg/kg/day) while no effects on offspring were noted. For CAS RN 124-30-1, reproductive organs were examined in both two-year toxicity studies with rats and the one-year toxicity study with dogs. No effects were seen in the reproductive organs at the highest doses tested (approximately 25 mg/kg/day for rats and 15 mg/kg/day for dogs). Reproductive organs were examined in the 13-week dietary study with CAS RN 4088-22-6. The identification of 'foamy macrophages' in the ovaries of this study precludes a definition of a NOAEL. This finding is not considered related to reproductive toxicity per se and is likely related to clearance of the test material. However, finding these macrophages in the ovaries is not common for chemicals that have this type of lesion due to clearance. No effect on reproductive organs was observed in a 13-week dermal study with rabbits at 5 or 50 mg/kg/day. Reproductive and developmental screening for CAS RN 61790-33-8 was conducted in a study that followed OECD 421 guidelines. The parental and offspring NOAEL was 12.5 mg/kg based on body weight effects at the mid dose of 50 mg/kg/day. The high dose of 120 mg/kg/day was lethal. No effects on reproduction or developmental toxicity were observed. Evaluations of reproductive organs were made for the animals in the two 90-day rat studies and the 90-day dog study (CAS RN 61791-44-

4) meeting the requirements for the HPV screening for reproductive effects. No effects were observed at the highest doses tested (approximately 450, 400 and 120 mg/kg/day, respectively).

For the mixture (CAS RN 3151-59-5 + 36505-83-6), Segment II (teratology) studies in rats and rabbits and a Segment III (perinatal) study in rats were identified. Maternal body weights were decreased in the Segment II study for rats (NOAEL = 6.0 mg/kg/day) and rabbits (NOAEL not established). No developmental toxicity was observed in these studies and no effects on offspring or mothers were observed in the Segment III study (NOAELs = 30 mg/kg/day). No teratogenic or developmental toxicity was observed in either study at the highest doses tested. Results for two developmental toxicity studies were available for the supporting chemical, CAS RN 112-90-3. The NOAEL for maternal toxicity in rats was 10 mg/kg/day and the corresponding value for rabbits was 3.0 mg/kg/day. No teratogenic or developmental toxicity was observed in either study at the highest doses tested (80 and 30 mg/kg/day, respectively). A developmental toxicity study for CAS RN 4088-22-6 with rabbits at doses of 50, 250 and 1000 mg/kg/day provided a maternal NOAEL of 50 mg/kg/day without showing fetal effects at 250 mg/kg/day. Fetal body weight effects were minimal in the high dose group. No teratogenicity was observed.

Summary – Human Health-Related Data

The available acute oral LD_{50} study for the propanamine derivative with the extensive data for the other supporting chemicals provides adequate evidence that the FND Ether Amines Category chemicals are only moderately to slightly toxic via this route and exposure period. Acute dermal studies for the supporting chemicals indicate these chemicals can be classified as minimally toxic. Acute inhalation studies did not result in deaths under normal exposure conditions for two chemicals. Repeated dose toxicity studies had similar NOAELs (12.5 to 50 mg/kg/day for rats and 3 or 13 mg/kg/day for dogs). Importantly because the highest exposure potential for some of the FND Ether Amines Category chemicals is via skin contact, a number of repeat dose dermal studies indicate the chemicals are highly irritating. Irritation of the products is well established for the HPV chemicals in the Category as well (company literature). This irritation helps provide added assurance that human exposure will be limited due to avoidance of the irritant effects. No clear organ-specific toxicity occurred in any of the repeat dose studies with the supporting chemicals in the FND Ether Amines Category. In addition, available data indicate that the FND Ether Amines Category chemicals are unlikely to be mutagenic and that they are not reproductive or developmental toxins.

Additional Testing – Human Health-Related Studies

In evaluating further testing of the FND Ether Amines Category chemicals, it is useful to review the available data for the related FND Cationic and FND Amides Category chemicals. Acute oral toxicity studies (approximately 80 studies for 40 chemicals in the three categories) provide LD_{50} values from approximately 400 to 10,000 mg/kg with no apparent organ specific toxicity. Similarly, repeated dose toxicity studies (approximately 35 studies for 15 chemicals) provide NOAELs between 10 and 100 mg/kg/day for rats and slightly lower for dogs. More than 60 genetic toxicity studies (*in vitro* bacterial and mammalian cells as well as *in vivo* studies) indicated only one equivocally positive Salmonella Reverse Mutation assay and one positive chromosomal aberration assay (this latter study ultimately shown to be aberrant), among more than 30 chemicals tested. For reproductive evaluations, 14 studies evaluated reproductive endpoints and/or reproductive organs for 11 chemicals, and 15 studies evaluated developmental toxicity for 13 chemicals, the evaluations indicating no reproductive or developmental effects for the FND group as a whole.

These comparisons clearly provide a strong weight of evidence that the FND Ether Amines Category chemicals will not pose significant toxicity to humans. As noted previously, the FND Ether Amines Category chemicals are very similar in structure and function. As outlined in Text Table C, the minimal difference among the alkyl substituents and the large database for the FND Categories indicates that the structural differences in these large alkyl chains do not result in differences in toxicity or mutagenicity. Thus, there is no scientifically justifiable expectation that the chemicals in the Category will result in significant toxicity not already established by tests with the HPV and supporting chemicals. Thus, based on this conclusion as well as the limited human exposure resulting from the use patterns and irritant properties, no additional testing is proposed for the FND Ether Amines Category chemicals. Table 7 provides the Test Plan for the human health related endpoints.

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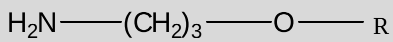
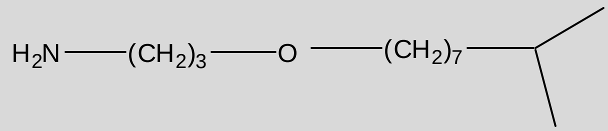
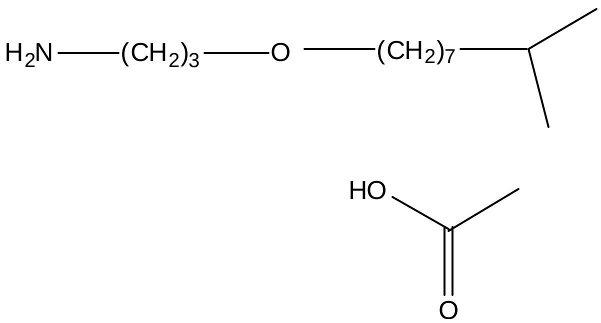
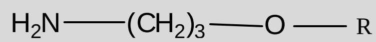
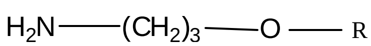
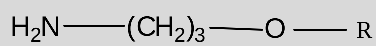
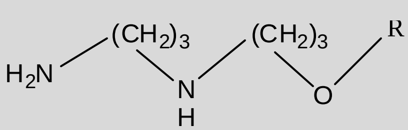
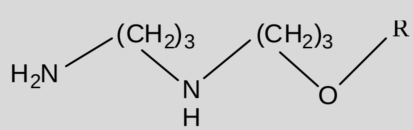
Table 1

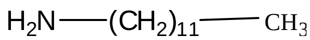
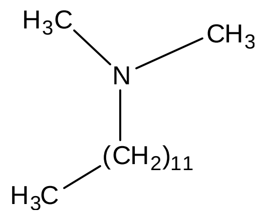
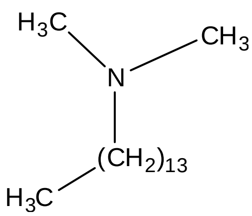
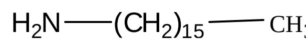
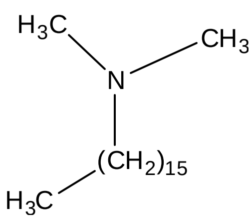
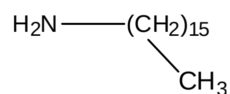
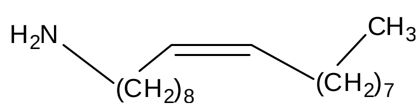
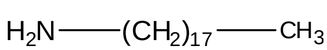
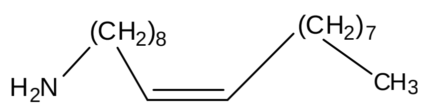
Structures of FND Ether Amines Category Chemicals

 **R = $C_8 – C_{10}$ alkyl** 1-Propanamine, 3-(C_{8-10}-alkyloxy) derivs 68784-38-3	 1-Propanamine, 3-(isodecyloxy)- 30113-45-2
 *1-Propanamine, 3-(isodecyloxy)-, acetate* *28701-67-9*	 **R = $C_9 – C_{11}$ isoalkyl, C_{10} rich** 1-Propanamine, 3-(C_{9-11}-isoalkyloxy)derivs., C_{10} rich 218141-16-3
 **R = C_{13} alkyl, branched** *1-Propanamine, 3-(tridecyloxy)-, branched* *68511-40-0*	 **R = $C_{11} – C_{14}$ isoalkyl, C_{13} rich** 1-Propanamine, 3-(C_{11-14}-isoalkyloxy)derivs., C_{13} rich 151789-06-9
 **R = C_{13} alkyl, branched** 1,3-Propanediamine, N-[3-(tridecyloxy)propyl]-, branched 68479-04-9	 **R = $C_{11} – C_{14}$-isoalkyl derivs., C_{13} rich** 1,3-propanediamine, N-(3-(C_{11-14}-isoalkyloxy)propyl)derivs, C_{13} rich 151789-07-0

Shaded cells indicate HPV-Sponsored FND Ether Amines Category chemicals

Table 1

Structures of FND Ether Amines Category Chemicals

 Dodecylamine 124-22-1	 *1-Dodecanamine, N,N-dimethyl* *112-18-5*
 1-Tetradecanamine, N,N-dimethyl 112-75-4	 Hexadecylamine 143-27-1
 1-Hexadecanamine, N,N-dimethyl 112-69-6	 *Hexadecylamine hydrofluoride (Hetaflur)*[3] *3151-59-5*  *9-Octadecen-1-amine hydrofluoride*[3] *36505-83-6*
 Octadecylamine 124-30-1	 *Cis-9-Octadecenylamine* *112-90-3*

[3] Hydrofluoride salt not shown in structure.

Table 1

Structures of FND Ether Amines Category Chemicals

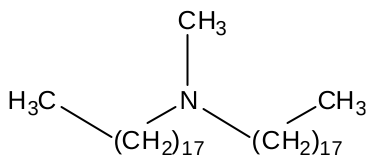
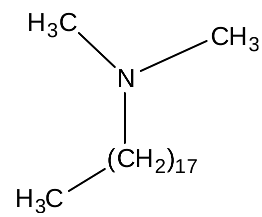
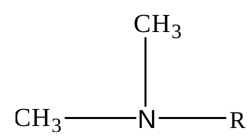
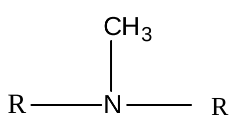
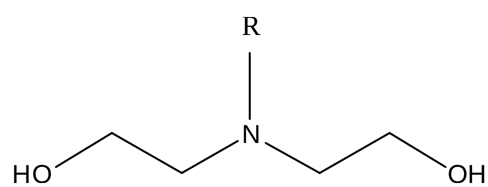
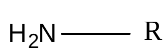
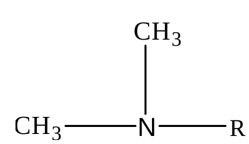
 1-Octadecanamine, N-methyl-N-octadecyl 4088-22-6	 1-Octadecanamine, N,N-dimethyl 124-28-7
 **R = coco alkyl** *Amines, coco alkyl* *61788-46-3*	 **R = coco alkyl** *Amines, coco alkyl dimethyl* *61788-93-0*
 **R = coco alkyl** *Amines, dicoco alkylmethyl* *61788-62-3*	 **R = coco alkyl derivs.** Ethanol, 2,2'-iminobis-, N-coco alkyl derivs. 61791-31-9
 **R = hydrogenated tallow alkyl** *Amines, hydrogenated tallow alkyl* *61788-45-2*	 **R = hydrogenated tallow alkyl** Amines, (hydrogenated tallow alkyl)dimethyl 61788-95-2

Table 1

Structures of FND Ether Amines Category Chemicals

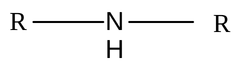
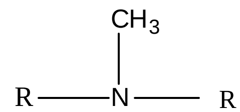
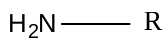
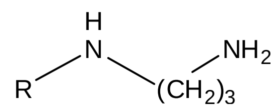
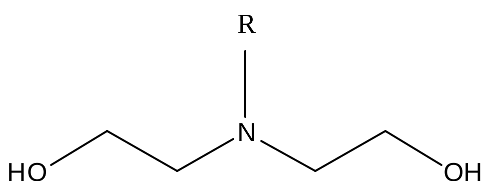
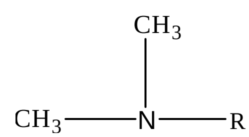
 **R = hydrogenated tallow alkyl** *Amines, bis(hydrogenated tallow alkyl)* *61789-79-5*	 **R = hydrogenated tallow alkyl** Dihydrogenated tallow methylamine 61788-63-4
 **R = tallow alkyl** *Amines, tallow alkyl* *61790-33-8*	 **R = tallow alkyl** Amines, N-tallow alkyltrimethylenedi- 61791-55-7
 **R = tallow alkyl derivs.** Ethanol, 2,2'-iminobis-, N-tallow alkyl derivs. 61791-44-4	 **R = soya alkyl** Amines, dimethyl soya alkyl 61788-91-8

Table 2

Physical/Chemical Properties Data for FND Ether Amines Category Chemicals

CAS RN	Melting Point (°C)	Boiling Point (°C)	Vapor Pressure (hPa)	Partition Coefficient (log K_{ow})	Water Solubility (mg/L)
68784-38-3					
30113-45-2	51	278	0.0035	3.92	165
28701-67-9					
218141-16-3					
68511-40-0	81	322	0.00017	5.40	5.38
151789-06-9					
68479-04-9	130	380	2.2×10^{-6}	5.37	2.64
151789-07-0					
124-22-1	**28.3** 28.3	**259** 259	0.0081	4.76	**2000** 45.1
112-18-5	**-15 to -20** 22	260	0.0159	5.44	8.58
112-75-4	43	292	0.0020	6.42	0.88
143-27-1	47	323	0.00013	6.73	0.48
112-69-6	63	321	0.00029	7.41	0.089
3151-59-5 + 36505-83-6					
124-30-1	**52.9** 52.9	**347** **349** 347	**0.000012** 0.000087	7.71	**1000** **not soluble** 0.049
112-90-3	**~21** **21** 93	**275- 344** **335** 346	**< 1.3** **0.00013** [4] 0.000037	**7.5** [4] **and 8.1** [4] **7.5** [4] **>3.11** 7.50	**(0.5×10^{-3})** [4] **and** **(0.7×10^{-5})** [4] **insoluble** **very insoluble** 0.076

[4] Estimated value.

Table 2

Physical/Chemical Properties Data for FND Ether Amines Category Chemicals

CAS RN	Melting Point (°C)	Boiling Point (°C)	Vapor Pressure (hPa)	Partition Coefficient (log K_{ow})	Water Solubility (mg/L)
4088-22-6	216	543	2.0 E-11	17	2.2 E-11
124-28-7	**22.9** **19.6 - 22.4** 22.9	346	0.00017	8.39	**not soluble** 0.009
61788-46-3					
61788-93-0					
61788-62-3					
61791-31-9					
61788-45-2	**52.9** 52.9	**348** 347	**0.000012** 0.000087	7.71	0.049
61788-95-2					
61789-79-5					
61788-63-4				**3.15**	**0.288**
61790-33-8	**34 – 40** **25 – 30**	**200 – 230**	**< 1.3**	**7.5**	**insoluble**
61791-55-7					
61791-44-4					
61788-91-8					

Note: Bold font indicates reliable data for which a Robust Summary is provided in Appendix A.
Regular font indicates data obtained from appropriate models as described in the text and Appendix B.
Shaded cells are the HPV-sponsored FND Ether Amines Category chemicals.
Empty block denotes data either are not available or are available and judged inadequate.

Table 3

Environmental Fate and Ecotoxicity Data for FND Ether Amines Category Chemicals

CAS RN	Photodegradation (cm^3/molecule-sec for k_{phot})	Stability in Water	Transport & Distribution [5]	Biodegradation	Acute/Prolonged Toxicity to Fish 96-hour LC_{50} (mg/L)	Acute/Chronic Toxicity to Invertebrates EC_{50} (mg/L)	Toxicity to Aquatic Plants 72-hr. EC_{50} (mg/L)
68784-38-3							
30113-45-2	64 E-12 $t_{1/2}$ = 2.0 hr	not calculable	Air: <1% Water: 90% Soil: <1% Sediment: 10%	**45% in 28 d**	126 (3.5) [6]	7.9 (0.33) [6]	not calculable (1.21) [6]
28701-67-9				**51% in 28 d**			
218141-16-3							
68511-40-0	68 E-12 $t_{1/2}$ = 1.9 hr	not calculable	Air: <1% Water: 26% Soil: <1% Sediment: 74%		not toxic at solubility	3.24 (0.05) [6]	not calculable (0.33) [6]
151789-06-9							
68479-04-9	154 E-12 $t_{1/2}$ = 0.8 hr	not calculable	Air: <1% Water: 27% Soil: <1% Sediment: 73%		**0.16** not toxic at solubility	**LC_{50} = 0.132** not toxic at solubility (0.07) [6]	not calculable (0.42) [6]
151789-07-0							
124-22-1	46 E-12 $t_{1/2}$ = 2.8 hr	not calculable	Air: <1% Water: 75% Soil: <1% Sediment: 25%	**> 60% ThOD in 28 d**	**0.42** 9.77 (0.87) [6]	3.24 (0.09) [6]	not calculable (0.45) [6]

[5] Water was assumed to be the exclusive route of entry into the environment.

[6] Original model calculations were made specifying the chemicals as "Cationic Surfactants"; a second calculation was made assuming the chemicals are Aliphatic Amines – the values for this second calculation are included in ( ) if different than for Cationic Surfactants.

Table 3

Environmental Fate and Ecotoxicity Data for FND Ether Amines Category Chemicals

CAS RN	Photodegradation (cm^3/molecule-sec for k_{phot})	Stability in Water	Transport & Distribution [5]	Biodegradation	Acute/Prolonged Toxicity to Fish 96-hour LC_{50} (mg/L)	Acute/Chronic Toxicity to Invertebrates EC_{50} (mg/L)	Toxicity to Aquatic Plants 72-hr. EC_{50} (mg/L)
112-18-5	93 E-12 $t_{1/2}$ = 1.4 hr	not calculable	Air: <1% Water: 42% Soil: <1% Sediment: 58%	**67% ThOD in 28 d** **72% TCO_2 in 29 d** **67% ThN-BOD in 28 d**	**0.57** not toxic at solubility	**0.083** 3.24 (0.04) [7]	**E_bC_{50}.= 0.056** [8] **E_rC_{50}.= 0. 092** **E_bC_{50}.= 0.034** **E_rC_{50}.= 0.056** **E_bC_{50} 0.0133** **E_rC_{50} 0.0235** not calculable (0.26) [7]
112-75-4	96 E-12 $t_{1/2}$ = 1.3 hr	not calculable	Air: <1% Water: 7% Soil: <1% Sediment: 93%	**$\leq$ 2% COD in 28 d** [9]	**0.18** **> 0.01 and < 1.0** **>0.01 and < 0.1** **0.35** not toxic at solubility	not toxic at solubility (0.01) [7]	not calculable (not toxic at solubility) [7]
143-27-1	51 E-12 $t_{1/2}$ = 2.5 hr	not calculable	Air: <1% Water: 13% Soil: <1% Sediment: 87%		not toxic at solubility	not toxic at solubility (0.008) [7]	not calculable (not toxic at solubility) [7]

[7] Original model calculations were made specifying the chemicals as “Cationic Surfactants”; a second calculation was made assuming the chemicals are Aliphatic Amines – the values for this second calculation are included in ( ) if different than for Cationic Surfactants.
[8] First four values are from a single study using two natural water sources.
[9] The scientific validity of this value is unjustifiable based on all other tests of similar chemicals. The assay is presumed to be invalid.

Table 3

Environmental Fate and Ecotoxicity Data for FND Ether Amines Category Chemicals

CAS RN	Photodegradation (cm^3/molecule-sec for k_{phot})	Stability in Water	Transport & Distribution [5]	Biodegradation	Acute/Prolonged Toxicity to Fish 96-hour LC_{50} (mg/L)	Acute/Chronic Toxicity to Invertebrates EC_{50} (mg/L)	Toxicity to Aquatic Plants 72-hr. EC_{50} (mg/L)
112-69-6	99 E-12 $t_{1/2}$ = 1.3 hr	not calculable	Air: <1% Water: 5% Soil: <1% Sediment: 95%	**59% ThOD in 28 d (70% in 42 d)** **107% TCO_2 in 29 d**	**0.18** **>0.1 and <1.0** not toxic at solubility	not toxic at solubility	not calculable (not toxic at solubility) [7]
3151-59-5 + 36505-83-6							
124-30-1	54 E-12 $t_{1/2}$ = 2.4 hr	not calculable	Air: <1% Water: 10% Soil: <1% Sediment: 90%	**>60% ThOD in 12 d** **70% ThOD in 28 d**	not toxic at solubility	**0.13** not toxic at solubility	**E_bC_{50} = 0.062** **E_rC_{50} =0.12** not calculable (not toxic at solubility) [10]
112-90-3	110 E-12 $t_{1/2}$ = 1.2 hr	not calculable	Air: <1% Water: 11% Soil: <1% Sediment: 89%	**> 60% ThOD in 12 d** **44% ThOD in 28 d (72% in 42 d)** **66% $ThC0_2$ in 28 d** **69% ThOD in 28 d**	**0.11** not toxic at solubility	**0.011** not toxic at solubility	**96-hour:** **E_bC_{50} =0.03** **E_rC_{50} =0.04** not calculable (not toxic at solubility) [10]
4088-22-6	134 E-12 $t_{1/2}$ = 1.0 hr	not calculable	Air: <1% Water: 5% Soil: <1% Sediment: 95%		**>100 and <500** [11] not toxic at solubility	not toxic at solubility	not calculable (not toxic at solubility) [10]

[10] Original model calculations were made specifying the chemicals as "Cationic Surfactants"; a second calculation was made assuming the chemicals are Aliphatic Amines – the values for this second calculation are included in ( ) if different than for Cationic Surfactants.
[11] The value(s) is(are) questionable due to the bioavailability of the test substance in this study.

Table 3

Environmental Fate and Ecotoxicity Data for FND Ether Amines Category Chemicals

CAS RN	Photodegradation (cm^3/molecule-sec for k_{phot})	Stability in Water	Transport & Distribution [5]	Biodegradation	Acute/Prolonged Toxicity to Fish 96-hour LC_{50} (mg/L)	Acute/Chronic Toxicity to Invertebrates EC_{50} (mg/L)	Toxicity to Aquatic Plants 72-hr. EC_{50} (mg/L)
124-28-7	102 E-12 $t_{1/2}$ = 1.3 hr	Not calculable	Air: <1% Water: 5% Soil: <1% Sediment: 95%	**91% TCO_2 at 0.2 mg/L in 7 d (79% at 2.0 mg/L in 7 d); 118% TCO_2 at 10 mg/L in 40 d; and 51% TCO_2 at 20 mg/L in 40 d** **49% TCO_2 in 28 d**	**0.18** **>0.1 and <1.0** not toxic at solubility	**LC_{50} = 0.074** [12] not toxic at solubility	**0.029; 0.11** **> 0.032; 0.16** [13] not calculable (not toxic at solubility) [14]
61788-46-3				**56% ThOD in 28 d (74% in 42 d)** **58% $ThC0_2$ in 28 d** **91.1% $ThC0_2$ in 28 d**	**0.16** **0.24**	**0.045** **0.09** **Larvae = 2.0 – 3.0** [15] **Pupae = 3.5 – 13.0** [15]	**E_bC_{50} = 0.14** **E_rC_{50} = 0.17** **96-hour:** **E_bC_{50} =0.00075** **E_rC_{50} =0.0011**
61788-93-0				**81% ThOD in 28 d** **69% ThOD in 28 d**	**>0.1 and <1.0**		
61788-62-3				**82% ThOD in 28 d**	**6.15**		

[12] 96-hour LC_{50} value for *Mysidopsis bahia*

[13] The study was conducted on *Selenastrum capricornutum* and *Microcystis aeruginosa* with a 5-day exposure and a 9-day recovery period. First two values are the algistatic concentrations for each species, respectively. Second two values are the algicidal concentrations for each species. An EC_{50} was not determined.

[14] Original model calculations were made specifying the chemicals as "Cationic Surfactants"; a second calculation was made assuming the chemicals are Aliphatic Amines – the values for this second calculation are included in ( ) if different than for Cationic Surfactants.

[15] Values are ppm. Test performed on 4 strains of mosquito larvae and pupae; *C .p. quinquefasciatus, A. albimanus, A. aegypti*, and *A. nigromaculis.*

Table 3

Environmental Fate and Ecotoxicity Data for FND Ether Amines Category Chemicals

CAS RN	Photodegradation (cm^3/molecule-sec for k_{phot})	Stability in Water	Transport & Distribution [5]	Biodegradation	Acute/Prolonged Toxicity to Fish 96-hour LC_{50} (mg/L)	Acute/Chronic Toxicity to Invertebrates EC_{50} (mg/L)	Toxicity to Aquatic Plants 72-hr. EC_{50} (mg/L)
61791-31-9				**61% COD in 28 d (62% in 42 d); Up to 85% TCO_2 in 28 d – Activated Sludge; >97% SCAS Removal; 100% (River Die Away)**	**0.47 (48-hour)** **0.0179 (30-day)**	**0.38 (48-hour)** **0.15 (21-day growth)** **0.14 (21-day growth)**	
61788-45-2	54 E-12 $t_{1/2}$ = 2.4 hr	not calculable	Air: <1% Water: 10% Soil: <1% Sediment: 90%	**75% ThOD in 28 d** **64% CO_2 in 28 d**	**0.88** not toxic at solubility	**0.16** **<1.0** not toxic at solubility	**96-hour:** **E_bC_{50} [16] = 0.012** **E_rC_{50} [16] ~ 0.016** not calculable (not toxic at solubility) [17]
61788-95-2				**58% ThOD in 28d (66% in 42 d)**			
61789-79-5				**16% O_2 in 28 d [18]**	**220 and 500[18]**		

[16] E_bC_{50} is the EC_{50} based on growth (biomass); E_rC_{50} is the EC_{50} based on growth rate.
[17] Original model calculations were made specifying the chemicals as "Cationic Surfactants"; a second calculation was made assuming the chemicals are Aliphatic Amines – the values for this second calculation are included in ( ) if different than for Cationic Surfactants.
[18] The value(s) is(are) questionable due to the bioavailability of the test substance in this study.

Table 3

Environmental Fate and Ecotoxicity Data for FND Ether Amines Category Chemicals

CAS RN	Photodegradation (cm^3/molecule-sec for k_{phot})	Stability in Water	Transport & Distribution [5]	Biodegradation	Acute/Prolonged Toxicity to Fish 96-hour LC_{50} (mg/L)	Acute/Chronic Toxicity to Invertebrates EC_{50} (mg/L)	Toxicity to Aquatic Plants 72-hr. EC_{50} (mg/L)
61788-63-4				75% ThOD in 28 d (85% in 40 d); 100% COD in 28 d; 48.3 or 63.5% in 53 d; 78.5 or 73.0% in 55 d; 70.47% in 28 d (acclimated sludge); 91.2% SCAS Removal	>1000 [19] 23 180	35.2 (48-hr acute)[19] 790 (48-hr acute)[19] 3.1 (48-hr acute) 21 (48-hr acute) 2.0 (48-hr acute) 6.5; 22; 60 (48-hour acute) [20]	E_bC_{50}= 0.05 E_rC_{50} = 0.12 AC_{d5} = 0.052 AC_{d5} = 0.96 AC_{d5} = 4.6 AC_{d5} = 1.14 [21]
61790-33-8				56% TCO_2 in 28 d >51% BOD in 28 d (~70% in 42 d) 73% in 28 d	9.3 >0.18 and <0.25	0.093 0.09 <0.25	E_bC_{50} = 0.052 E_rC_{50} =0.059 E_bC_{50} = 0.068 E_rC_{50} =0.083
61791-55-7				90% DOC elimination in 3 hrs; 87% adsorption in sludge			

[19] The value(s) is(are) questionable due to the bioavailability of the test substance in this study.

[20] Three studies with a mixture or a prill containing the test substance were conducted in different source waters – EC_{50} values are as the mixture/prill concentration; well water with mixture EC_{50} = 6.5 mg/L (83.5% ditallowmethylamine); well water with prill EC_{50} = 22 mg/L (63% ditallowmethylamine); river water with prill EC_{50} = 60 mg/L (63% ditallowmethylamine).

[21] AC_{d5} = Algistatic concentration after 5 days exposure. Four separate studies were conducted on four strains of algae; *Selenastrum capricornutum, Microcystis aeruginosa, Navicula seminulum,* and *Navicula pelliculosa.*

Table 3

Environmental Fate and Ecotoxicity Data for FND Ether Amines Category Chemicals

CAS RN	Photodegradation (cm^3/molecule-sec for k_{phot})	Stability in Water	Transport & Distribution [5]	Biodegradation	Acute/Prolonged Toxicity to Fish 96-hour LC_{50} (mg/L)	Acute/Chronic Toxicity to Invertebrates EC_{50} (mg/L)	Toxicity to Aquatic Plants 72-hr. EC_{50} (mg/L)
61791-44-4				**52% ThOD in 28 d (62% in 35 d)**			
61788-91-8				**98% ThOD in 28 d**	**> 0.1 and < 1.0**		

Note: Bold font indicates reliable data for which a Robust Summary is provided in Appendix A.
Regular font indicates data obtained from appropriate models as described in the text and Appendix B.
Shaded cells are the HPV-sponsored FND Ether Amines Category chemicals.
Empty block denotes data either are not available or are available and judged inadequate.

Table 4

Human Health-Related Data for FND Ether Amines Category Chemicals

CAS RN	Acute Oral Toxicity (g/kg)	Acute Inhalation Toxicity (mg/L)	Acute Dermal Toxicity (g/kg)	Repeated Dose Toxicity NOAEL (mg/kg/day)	Genetic Toxicity *In vitro/ In vivo*	Toxicity to Reproduction NOAEL (mg/kg/day)	Developmental Toxicity NOAEL (mg/kg/day)
68784-38-3							
30113-45-2							
28701-67-9	1.46 (male) 1.03 (female)				Negative (Ames)		
218141-16-3							
68511-40-0					Negative (Ames)		
151789-06-9							
68479-04-9							
151789-07-0							
124-22-1	1.02 1.16 (mouse) >2.0						
112-18-5	1.22 0.79 >1.26 and <2.52		~5.0		Negative (*in vivo* mouse micronucleus)		
112-75-4	2.116 1.32				Negative (Ames) [22]		
143-27-1					Negative (Ames) Negative (Ames)		
112-69-6	0.80 ml/kg >2.0 1.015		4.29 ml/kg		Negative (Ames) [22]		

[22] Evaluation with only two tester strains.

Table 4

Human Health-Related Data for FND Ether Amines Category Chemicals

CAS RN	Acute Oral Toxicity (g/kg)	Acute Inhalation Toxicity (mg/L)	Acute Dermal Toxicity (g/kg)	Repeated Dose Toxicity NOAEL (mg/kg/day)	Genetic Toxicity *In vitro/ In vivo*	Toxicity to Reproduction NOAEL (mg/kg/day)	Developmental Toxicity NOAEL (mg/kg/day)
3151-59-5 + 36505-83-6				6.0 [23] 6.0 [24]		Parents =6.0 Offspring = 30.0 [25]	Maternal = 6.0 Developmental = 30.0 [26] Maternal LOAEL = 1.2 Developmental = 30.0 [27] Maternal and Offspring = 30.0 [28]
124-30-1	~1.0 (rat and mouse) >2.0 >2.0			~25 [29] ~25 [30] 3.0 [31]	Negative (Ames) Negative (Ames) Negative (Ames)	~25 [29] ~25 [30] 15 [31]	
112-90-3	~2.0 (females) ~ 1.18 (males)			See Robust Summary [32]	Negative (Ames) Negative (gene mutation) Negative (mouse lymphoma) Negative (chrom. aberration) Negative (*in vivo* cytogenetic)		Maternal = 10; Developmental = 80 [33] Maternal =3.0 ; Developmental =30 [34]

[23] 24-Month feeding study in rats at doses of 1.2, 6.0 and 30.0 mg/kg/day.
[24] Two-year study in dogs via oral gavage at doses of 1.2, 6.0 and 12.0 mg/kg/day.
[25] Segment I (Fertility and General Reproductive Performance) study in rats via oral gavage at doses of 1.2, 6.0 and 30.0 mg/kg/day.
[26] Two Segment II (Teratology) studies in rats were conducted at doses of 1.2, 6.0 and 30.0 mg/kg/day. Decreases in maternal body weight gains at 30.0 mg/kg/day in the confirmatory study.
[27] Segment II (Teratology) study in rabbits at doses of 1.2, 6.0 and 30.0 mg/kg/day. Maternal body weight decreased at the low dose.
[28] Segment III (Perinatal and Postnatal) study in rats at doses of 1.2, 6.0 and 30.0 mg/kg/day.
[29] Chronic (two-year) dietary toxicity study in rats. The NOAEL was 500 ppm (highest dose tested) estimated to be approximately 25 mg/kg/day. Reproductive organs were examined, meeting the requirements for SIDS/HPV reproductive screening.
[30] Chronic (two-year) dietary toxicity study in rats. Reproductive organs were examined, meeting the requirements for SIDS/HPV reproductive screening.
[31] Chronic (one-year) oral (capsule) toxicity study in dogs. Reproductive organs were examined, meeting the requirements for SIDS/HPV reproductive screening.
[32] A 14-day dermal toxicity study in rats with limited evaluations; not adequate for SIDS/HPV testing but provides data on the irritation of the chemical following repeated exposure.
[33] Developmental toxicity study in rats dosed via oral gavage at doses of 0, 10, 40 and 80 mg/kg.
[34] Developmental toxicity study in rabbits dosed via oral gavage at doses of 0, 3, 10 and 30 mg/kg/day.

Table 4

Human Health-Related Data for FND Ether Amines Category Chemicals

CAS RN	Acute Oral Toxicity (g/kg)	Acute Inhalation Toxicity (mg/L)	Acute Dermal Toxicity (g/kg)	Repeated Dose Toxicity NOAEL (mg/kg/day)	Genetic Toxicity *In vitro/ In vivo*	Toxicity to Reproduction NOAEL (mg/kg/day)	Developmental Toxicity NOAEL (mg/kg/day)
4088-22-6	>2.0 >5.0		>2.0	LOAEL = 130 [35] LOAEL = 100 [36] LOAEL = 50 [37] LOAEL = 5 [38]	Negative (Ames)	LOAEL = 130 [35] LOAEL = 50 [38]	Maternal = 50 Developmental = 250
124-28-7	0.78 ml/kg 2.116		4.29 ml/kg		Negative (Ames) [39]		
61788-46-3	1.24 (male) 1.39 (female) >2.0 (male) 2.82 (female) 2.04 >6.0	>0.099 [40]	>2.0 (rat) >2.0 ml/kg >2.0 ml/kg		Negative (Ames)		
61788-93-0	1.50 (male) 1.30 (female); >1.0 and <1.25 1.58 ml/kg		4.29 ml/kg				
61788-62-3	>2.0						
61791-31-9	>5.0						
61788-45-2	>5.0 4.8 >2.0						
61788-95-2	>2.0						
61789-79-5	>10.0 (males)						

35 13-week dietary toxicity study in rats. Reproductive organs were examined, meeting the requirements for SIDS/HPV reproductive screening.
36 4-week gavage range-finding study (developmental toxicity) in rabbits
37 7-day dermal range finding study in rabbits; LOAEL determined by skin irritation
38 13-week dermal study in rabbits (5 and 50 mg/kg/day); LOEL for repeated dose toxicity determined by skin irritation. Reproductive organs were examined, meeting the requirements for SIDS/HPV reproductive screening.
39 Evaluation in only two tester strains.
40 Exposure period = 1 hour

Table 4

Human Health-Related Data for FND Ether Amines Category Chemicals

CAS RN	Acute Oral Toxicity (g/kg)	Acute Inhalation Toxicity (mg/L)	Acute Dermal Toxicity (g/kg)	Repeated Dose Toxicity NOAEL (mg/kg/day)	Genetic Toxicity *In vitro/ In vivo*	Toxicity to Reproduction NOAEL (mg/kg/day)	Developmental Toxicity NOAEL (mg/kg/day)
61788-63-4	>5.0 >15.0				Negative (Ames) Negative (Mouse Lymphoma) Negative (*in vitro* UDS) Negative (*in vivo* Cytogenetics)		
61790-33-8	>2.50 (male) >2.00 (female); 2.23 ml/kg (male) 2.61 ml/kg (female)			12.5 [41]	Negative (Ames) Negative (*in vivo* rat micronucleus)	Parents = 12.5 Offspring = 12.5 [42]	Parents = 12.5 Offspring = 12.5 [42]
61791-55-7	>5.0						

[41] Four-week oral (gavage) toxicity study in rats.
[42] OECD 421 oral gavage study in rats.

Table 4

Human Health-Related Data for FND Ether Amines Category Chemicals

CAS RN	Acute Oral Toxicity (g/kg)	Acute Inhalation Toxicity (mg/L)	Acute Dermal Toxicity (g/kg)	Repeated Dose Toxicity NOAEL (mg/kg/day)	Genetic Toxicity *In vitro/ In vivo*	Toxicity to Reproduction NOAEL (mg/kg/day)	Developmental Toxicity NOAEL (mg/kg/day)
61791-44-4	1.50 (male) 1.20 (female) >2.0 0.89 0.63 1.15 >15.0		>2.0 ml/kg >2.0 <2.0 ml/kg [43] >1.5	~50 [44] 13 [45] 12 [46] 40/200 [47] 40 [48] 10 [49] 10 [50]	Negative (Ames) – 3 tests; Negative (Mouse Lymphoma) Negative without metabolic activation, Positive with metabolic activation (*in vitro* Chromosomal Aberration); Negative (*in vitro* UDS); Negative (Mouse Micronucleus); Negative (*in vivo* Cytogenetics)	~450 [44] 120 [45] 400 [46]	
61788-91-8	0.835 ml/kg		3.0 ml/kg				

Note: Shaded cells are the HPV-sponsored FND Ether Amines Category chemicals.
Empty block denotes data either are not available or are available and judged inadequate.

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[43] Four of 6 animals died following a 24-hour exposure to 2.0 ml/kg

[44] 90-day dietary toxicity study in rats. NOAEL for repeated dose toxicity was 500 ppm in the diet estimated to be approximately 50 mg/kg/day. Reproductive organs were examined, meeting the requirements for SIDS/HPV reproductive screening. NOAEL for repeated dose toxicity was 4500 ppm in the diet estimated to be approximately 450 mg/kg/day.

[45] 90-day dietary toxicity study in dogs. Doses of 40 and 120 mg/kg/day were poorly tolerated with extensive emesis. Reproductive organs were examined, meeting the requirements for SIDS/HPV reproductive screening.

[46] 13-week dietary study in rats. Reproductive organs were examined, meeting the requirements for SIDS/HPV reproductive screening.

[47] 28-day dermal study in rabbits (200 mg/kg/day for two days reduced to 40 mg/kg/day). Only skin irritation considered to be treatment related.

[48] 28-day dermal study in rabbits (only one dose tested; no systemic toxicity; skin irritation observed)

[49] 4-week dermal study in rabbits (two doses tested; no systemic toxicity; skin irritation observed for both the 2 and 10 mg/kg/day groups)

[50] 17-day dermal exposure in rabbits followed by approximately 10 weeks of examination (study terminated due to irritation of the 2 and 10 mg/kg/day doses)

Table 5

Proposed Test Plan for American Chemistry Council FND Ether Amines Category Physical/Chemical Properties

CAS RN	Melting Point (°C)	Boiling Point (°C)	Vapor Pressure (hPa)	Partition Coefficient (log K_{ow})	Water Solubility (mg/L)
68784-38-3	R	R	R	R	R
30113-45-2	M	M	M	M	M
28701-67-9	R	R	R	R	R
218141-16-3	R	R	R	R	R
68511-40-0	M	M	M	M	M
151789-06-9	R	R	R	R	R
68479-04-9	M	M	M	M	M
151789-07-0	R	R	R	R	R
124-22-1	**A** (M)	**A** (M)	M	M	**A** (M)
112-18-5	**A** (M)	M	M	M	M
112-75-4	M	M	M	M	M
143-27-1	M	M	M	M	M
112-69-6	M	M	M	M	M
3151-59-5 + 36505-83-6	R	R	R	R	R
124-30-1	**A** (M)	**A** (M)	**A** (M)	M	**A** (M)
112-90-3	**A** (M)	**A** (M)	**A** (M)	**A** (M)	**A** (M)
4088-22-6	M	M	M	M	M
124-28-7	**A** (M)	M	M	M	**A** (M)
61788-46-3	R	R	R	R	R
61788-93-0	R	R	R	R	R
61788-62-3	R	R	R	R	R
61791-31-9	R	R	R	R	R
61788-45-2	**A** (M)	**A** (M)	**A** (M)	M	M
61788-95-2	R	R	R	R	R
61789-79-5	R	R	R	R	R
61788-63-4	R	R	R	**A**	**A**

Table 5

Proposed Test Plan for American Chemistry Council FND Ether Amines Category Physical/Chemical Properties

CAS RN	Melting Point (°C)	Boiling Point (°C)	Vapor Pressure (hPa)	Partition Coefficient (log K_{ow})	Water Solubility (mg/L)
61790-33-8	**A**	**A**	**A**	**A**	**A**
61791-55-7	R	R	R	R	R
61791-44-4	R	R	R	R	R
61788-91-8	R	R	R	R	R

Note: Shaded cells are the HPV-sponsored FND Ether Amines Category chemicals.
A = Adequate reported values
M = Adequate model data available
R = Read across from available data and/or experimental determination is considered inappropriate.

Table 6

Proposed Test Plan for American Chemistry Council FND Ether Amines Category Environmental Fate and Ecotoxicity

CAS RN	Photodegradation (cm^3/molecule-sec for k_{phot})	Stability in Water	Transport & Distribution	Biodegradation	Acute/Prolonged Toxicity to Fish 96-hour LC_{50} (mg/L)	Acute/Chronic Toxicity to Invertebrates EC_{50} (mg/L)	Toxicity to Aquatic Plants 72-hr. EC_{50} (mg/L)
68784-38-3	R	R	R	R	R	R	R
30113-45-2	M	NC	M	**A**	M	M	M
28701-67-9	R	R	R	**A**	R	R	R
218141-16-3	R	R	R	R	R	R	R
68511-40-0	M	NC	M	R	M	M	M
151789-06-9	R	R	R	R	R	R	R
68479-04-9	M	N	M	R	**A** (M)	**A** (M)	M
151789-07-0	R	R	R	R	R	R	R
124-22-1	M	NC	M	**A**	**A** (M)	M	M
112-18-5	M	NC	M	**A**	**A** (M)	**A** (M)	**A** (M)
112-75-4	M	NC	M	**A**	**A** (M)	M	M
143-27-1	M	NC	M	R	M	M	M
112-69-6	M	NC	M	**A**	**A** (M)	M	M
3151-59-5 + 36505-83-6	R	R	R	R	R	R	R
124-30-1	M	NC	M	**A**	**M**	**A** (M)	**A** (M)
112-90-3	M	NC	M	**A**	**A** (M)	**A** (M)	**A** (M)
4088-22-6	M	NC	M	R	**A** (M)	M	M
124-28-7	M	NC	M	**A**	**A** (M)	**A** (M)	**A** (M)
61788-46-3	R	R	R	**A**	**A**	**A**	**A**
61788-93-0	R	R	R	**A**	**A**	R	R
61788-62-3	R	R	R	**A**	**A**	R	R
61791-31-9	R	R	R	**A**	**A**	**A**	R
61788-45-2	M	NC	M	**A**	**A** (M)	**A** (M)	**A** (M)
61788-95-2	R	R	R	**A**	R	R	R
61789-79-5	R	R	R	**A**	**A**	R	R
61788-63-4	R	R	R	**A**	**A**	**A**	**A**
61790-33-8	R	R	R	**A**	**A**	**A**	**A**

Table 6

Proposed Test Plan for American Chemistry Council FND Ether Amines Category Environmental Fate and Ecotoxicity

CAS RN	Photodegradation (cm^3/molecule-sec for k_{phot})	Stability in Water	Transport & Distribution	Biodegradation	Acute/Prolonged Toxicity to Fish 96-hour LC_{50} (mg/L)	Acute/Chronic Toxicity to Invertebrates EC_{50} (mg/L)	Toxicity to Aquatic Plants 72-hr. EC_{50} (mg/L)
61791-55-7	R	R	R	**A**	R	R	R
61791-44-4	R	R	R	**A**	R	R	R
61788-91-8	R	R	R	**A**	**A**	R	R

Note: Shaded cells are the HPV-sponsored FND Ether Amines Category chemicals.
A = Adequate reported values
M = Adequate model data available
R = Read across from available data and/or experimental determination is considered inappropriate.
NC = Model could not calculate a value.

Table 7
Proposed Test Plan for American Chemistry Council FND Ether Amines Category
Human Health-Related Data

CAS RN	Acute Oral Toxicity (g/kg)	Acute Inhalation Toxicity (mg/L)	Acute Dermal Toxicity (g/kg)	Repeated Dose Toxicity NOAEL (mg/kg/day)	Genetic Toxicity In vitro/ In vivo	Toxicity to Reproduction NOAEL (mg/kg/day)	Developmental Toxicity NOAEL (mg/kg/day)
68784-38-3	R	R	R	R	R	R	R
30113-45-2	R	R	R	R	R	R	R
28701-67-9	**A**	R	R	R	**A (Ames)**	R	R
218141-16-3	R	R	R	R	R	R	R
68511-40-0	R	R	R	R	**A (Ames)**	R	R
151789-06-9	R	R	R	R	R	R	R
68479-04-9	R	R	R	R	R	R	R
151789-07-0	R	R	R	R	R	R	R
124-22-1	**A**	R	R	R	R	R	R
112-18-5	**A**	R	**A**	R	**A (Cyto)**	R	R
112-75-4	**A**	R	R	R	**A (Ames)**	R	R
143-27-1	R	R	R	R	**A (Ames)**	R	R
112-69-6	**A**	R	**A**	R	**A (Ames)**	R	R
3151-59-5 + 36505-83-6	R	R	R	**A**	R	**A**	**A**
124-30-1	**A**	R	R	**A**	**A (Ames)**	**A**	R
112-90-3	**A**	R	R	R	**A (Both)**	R	**A**
4088-22-6	**A**	R	**A**	**A**	**A (Ames)**	**A**	**A**
124-28-7	**A**	R	**A**	R	**A**	R	R
61788-46-3	**A**	**A**	**A**	R	**A (Ames)**	R	R
61788-93-0	**A**	R	**A**	R	R	R	R
61788-62-3	**A**	R	R	R	R	R	R
61791-31-9	**A**	R	R	R	R	R	R
61788-45-2	**A**	R	R	R	R	R	R
61788-95-2	**A**	R	R	R	R	R	R
61789-79-5	**A**	R	R	R	R	R	R
61788-63-4	**A**	R	R	R	**A (Both)**	R	R
61790-33-8	**A**	R	R	**A**	**A (Both)**	**A**	**A**
61791-55-7	**A**	R	R	R	R	R	R

Table 7
Proposed Test Plan for American Chemistry Council FND Ether Amines Category
Human Health-Related Data

CAS RN	Acute Oral Toxicity (g/kg)	Acute Inhalation Toxicity (mg/L)	Acute Dermal Toxicity (g/kg)	Repeated Dose Toxicity NOAEL (mg/kg/day)	Genetic Toxicity In vitro/ In vivo	Toxicity to Reproduction NOAEL (mg/kg/day)	Developmental Toxicity NOAEL (mg/kg/day)
61791-44-4	**A**	R	**A**	**A**	**A**	**A**	R
61788-91-8	**A**	R	**A**	R	R	R	R

Note: Shaded cells are the HPV-sponsored FND Ether Amines Category chemicals.
Reliable data for acute toxicity by any of the three routes of exposure are considered adequate under the EPA HPV Challenge Program.
A = Adequate reliable data
R = Endpoint fulfilled by category read-across from existing or proposed test data.